Supporting Information

Conductive Polymer (PEDOT) Contacts on p-, n- and n^+-Si: The Effects of Silicon Surface Functionalization and PEDOT Conductivity on the Junction Behavior

Michael G. Walter,[⊥] Xueliang Liu, Leslie E. O'Leary,
Bruce S. Brunschwig, and Nathan S. Lewis*

[*] Prof. N. S. Lewis, Corresponding Author
Beckman Institute and Kavli Nanoscience Institute
Division of Chemistry and Chemical Engineering
California Institute of Technology
210 Noyes Laboratory, 127-72
Pasadena, CA 91125 (USA)
E-mail: nslewis@caltech.edu

S1. Supplementary Figures

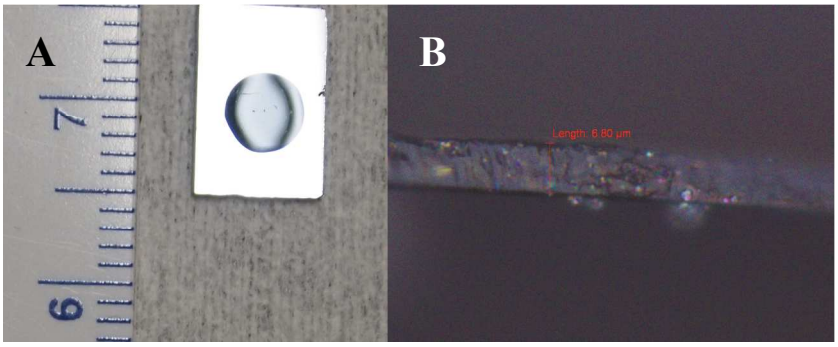

Figure S1. (a) Image of a dry PEDOT:PSS conductive polymer contact on an n-Si electrode. (b) Cross section of drop-cast PEDOT:PSS films (6.5±0.34 µm average thickness).

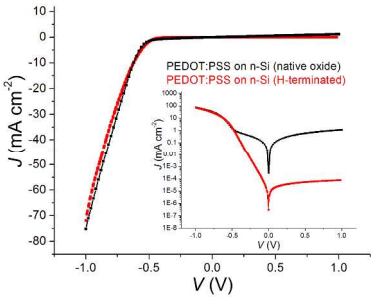

Figure S2. Comparison of the *J-V* behavior of PEDOT:PSS on a freshly etched n-Si surface, and an unetched n-Si surface that contained a native oxide.

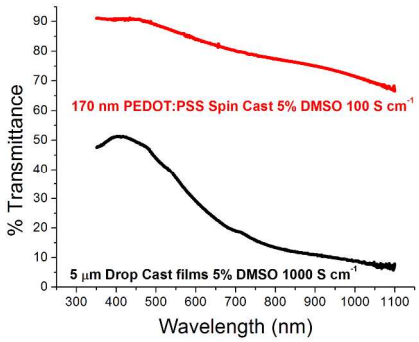

Figure S3. UV-visible transmittance of thick PEDOT:PSS drop cast films and thin spin-cast films on glass slides.

Calculated Bulk-recombination limited V_{oc} for PEDOT:PSS / n-Si junctions							
n-methyl Si			Device #	H-term Si			Device #
J_{sc}	V_{oc}	**Calc** recombination		J_{sc}	V_{oc}	**Calc** recombination	
28.74	609	604	56E	17.8	606	592	62B
18.12	590	592		12.1	593	582	
8.7	569	573		4.93	561	559	
28	600	604	62A	16.9	600	591	62C
17	587	591		11.5	580	581	
7	564	568		3.25	542	548	
10.82	584	585	56D			calc	
8.77	581	574					
4.36	560	556				62B 3 days later	
				5.19	557	559	

Table S1: Calculated bulk-recombination limited open-circuit voltages (V_{oc}) at various short-circuit current densities (J_{sc}) of both H-term and CH_3-terminated n-Si photoelectrodes using eq. 3

$$V_{oc} = \left(\frac{k_B T}{q}\right) \ln\left(\frac{J_{sc} L_p N_D}{n_i^2 \mu_p k_B T}\right)$$

$L_p = 2.0\text{x}10^{-2}$ cm, $n_i = 1.45\text{x}10^{10}$ cm^{-3}, $N_D = 1.04\text{x}10^{16}$ cm^{-3}, $\mu_p = 428$ cm^2 V^{-1} s^{-1}.